WHAT IS CLAIMED IS:

1. A method of modeling the behavior of a molecule, comprising

selecting a model for said molecule, said model having equations of motion for said molecule; and

integrating said model equations with an L-stable implicit integrator in large timesteps so as to obtain a calculations of said behavior of said molecule.

2. The method of claim 1 wherein said large timesteps comprise intervals of at least 200 femtoseconds.

3. The method of claim 2 wherein said integrating step is performed with varying timesteps.

4. The method of claim 1 further comprising

correcting for errors in said integrating step to obtain a history of states of said molecule over time.

5. The method of claim 1 wherein said selecting step includes selecting a stiff system model to obtain a history of states of said molecule over time.

6. The method of claim 1 wherein said integrating step includes avoiding energy conservation to obtain a minimum energy state for said molecule.

7. The method of claim 1 wherein said L-stable integrator comprises an integrator from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4, and other implicit Runge-Kutta methods.

8. The method of claim 3 further comprising

correcting for errors in said integrating step to obtain a history of states of said molecule over time.

9. The method of claim 3 wherein said selecting step includes selecting a stiff system model to obtain a history of states of said molecule over time.

10. The method of claim 3 wherein said integrating step includes avoiding energy conservation to obtain a minimum energy state for said molecule.

11. The method of claim 1 wherein said model is described in internal coordinates selected to speed calculations of said behavior of said molecule.

12. The method of claim 11 wherein said model comprises a torsion angle, rigid body model of said molecule

13. A method of modeling the behavior of a molecule, comprising

selecting a model for said molecule, said model having equations of motion for said molecule; and

selecting an L-stable integrator;

integrating said model equations with said L-stable integrator in timesteps of intervals varying over a range of at least 100 so as to obtain a calculation of said behavior of said molecule.

14. The method of claim 13 wherein said timesteps comprise intervals of at least 200 femtoseconds.

15. The method of claim 14 wherein said L-stable integrator is selected to remove energy from said model; and wherein said model equations are integrated without energy conservation to obtain a minimum energy state of said molecule.

16. The method of claim 15 wherein said L-stable integrator comprises an implicit Euler integrator.

17. The method of claim 14 wherein said model equations are integrated with error correction so as to obtain a history of states of said molecule over time.

18. The method of claim 14 wherein said model is selected for stiff equations of motion so as to obtain a history of states of said molecule over time.

19. The method of claim 14 wherein said model is selected for stiff equations of motion and said model equations are integrated with error correction, so as to obtain a history of states of said molecule over time.

20. The method of claim 19 wherein said L-stable integrator comprises a Radau5 integrator.

21. The method of claim 14 wherein said L-stable integrator is selected from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4 and implicit Runge-Kutta methods.

22. The method of claim 14 wherein said model is described in internal coordinates selected to speed calculations of said behavior of said molecule.

23. The method of claim 22 wherein said model comprises a torsion angle, rigid body model of said molecule.

24. A method of modeling the behavior of a first molecule with a plurality of second molecules, comprising

selecting a first model for said first molecule, said model having equations of motion for said first molecule;

selecting a second model for each of said second molecules, said model having equations of motion for said second molecule;

selecting an L-stable integrator;

integrating said model equations with said L-stable integrator in timesteps of intervals varying in a range of at least 100 so as to obtain a calculations of said behavior of said first molecule with said plurality of second molecules.

25. The method of claim 24 wherein said model equations are described in internal coordinates selected to speed calculations of said behavior.

26. The method of claim 24 wherein said second molecule is selected from the group comprising salts, solvents, and other organic and inorganic compounds.

27. The method of claim 26 wherein said second molecule comprises water.

28. The method of claim 25 wherein said first molecule comprises a protein.

29. The method of claim 25 wherein said large timesteps comprise intervals of at least 200 femtoseconds.

30. The method of claim 29 wherein said L-stable integrator is selected to remove energy from said model; and wherein said model equations are integrated without energy conservation to obtain a minimum energy state of said molecule.

31. The method of claim 30 wherein said L-stable integrator comprises an implicit Euler integrator.

32. The method of claim 25 wherein said model equations are integrated with error correction so as to obtain a history of states of said molecule over time.

33. The method of claim 25 wherein said model is selected for stiff equations of motion so as to obtain a history of states of said molecule over time.

34. The method of claim 25 wherein said model is selected for stiff equations of motion and said model equations are integrated with error correction, so as to obtain a history of states of said molecule over time.

35. Computer code for modeling the behavior of a molecule on a computer, said code comprising

a first module defining a model for said molecule, said model including equations of motion for said molecule and

a second module integrating said equations of motions with an L-stable implicit integrator to obtain calculations of said behavior of said molecule.

36. The computer code of claim 35 wherein said second module integrates said equations of motion with varying timesteps.

37. The computer code of claim 36 wherein said timesteps vary in magnitude over a range of at least 100.

38. The computer code of claim 35 wherein said first module defines said model with internal coordinates.

39. The computer code of claim 38 wherein said internal coordinates comprise generalized coordinates and generalized speeds.

40. The computer code of claim 39 wherein said first module defines a rigid multibody, torsion-angle model for said molecule.

41. A method of screening a library of compounds for interaction with a target, comprising

(a) selecting a model for the interaction of a compound with the target, the model having equations of motion for the compound and the target;

(b) inputting data for a first of the library of compounds into the equations of motions;

(c) integrating said model equations with an L-stable integrator in large time steps so as to obtain a calculation of the motions of the target and the compound and thereby the interaction of the compound with the target;

(d) repeating (b) and (c) for each compound in the library;

(e) comparing the interactions of the compounds with the target;

(f) synthesizing a compound selected based on its interaction with the target.

42. The method of claim 41, wherein the library of compounds comprises a lead compound known to interact with the target and test compounds to be tested for interaction with the target.

53. The method of claim 42, wherein the lead compound is a polypeptide and the test compounds are small molecules.

44. The method of claim 43, wherein the lead compound is an antibody.

45. The method of claim 42, wherein one of the compounds is a lead compound known to interact with the target and the comparing step compares the interactions between the test compounds and the target with that of the lead compound with the target to select a test compound having a similar interaction with the target to that of the lead compound.

46. The method of claim 42, further comprising identifying the lead compound from a primary library by contacting the lead compound with the target and detecting interaction between the lead compound and the target.

47. The method of claim 41, wherein different repetitions of steps (b) and (c) are performed on first and second compounds, the second compound being selected based on the interaction of the first compound with the target.

48. The method of claim 41, further comprising testing the synthesized compound for interaction with the target.

49. The method of claim 48, wherein the testing is performed in vitro, in a nonhuman animal or in a human.

50. The method of claim 41, further comprising formulating the synthesized compound as a pharmaceutical composition.

51. The method of claim 41, further comprising determining data relating to the structure of at least one of the library of compounds and/or the target.

52. The method of claim 51, wherein the data are determined by X-ray crystallography.

53. The method of claim 51, wherein the data are determined by infra red or ultraviolet spectroscopy, or NMR.

54. The method of claim 41, wherein the compounds are selected from the group consisting of proteins, nucleic acids, polysaccharides, phospholipids, hormones, prostaglandins, steroids, and small molecules.

55. The method of claim 54, wherein the compounds are small molecules selected from the group consisting of beta-turn mimetics, aromatic compounds, heterocyclic compounds, benzodiazepines, oligomeric N-substituted glycines and oligocarbamates.

56. The method of claim 41, wherein the target is selected from the group consisting of proteins, nucleic acids, carbohydrates, and lipids.

57. The method of claim 56, wherein the target is a receptor.

58. The method of claim 57, wherein the target is a membrane-bound receptor.

59. The method of claim 41, further comprising inputting data for a solvent or matrix containing the target and/or compound that interacts with the target into the equations of motion.

60. The method of claim 59, wherein the matrix is a phospholipid membrane.

61. The method of claim 41, wherein the solvent is an aqueous solvent.

62. The method of claim 41, wherein the solvent is an organic solvent.

63. The method of claim 41, wherein the data comprises the identity of components of the compound.

64. The method of claim 63, wherein the data comprises the identity of atoms of the compound.

65. The method of claim 41, wherein the data comprises X-ray crystallographic data.

66. The method of claim 41, further comprising inputting an environmental factor into the equations of motion.

67. The method of claim 41, wherein the environmental factor is the temperature or pressure at which interaction between the compound and target is to be determined.

68. The method of claim 41, wherein the library of compounds comprises at least 10^{10} members.

69. The method of claim 41, wherein the library of compounds comprises at least 10^{50} members.

70. The method of claim 41, wherein the integrating step determines a binding affinity between the compound and the target and the comparing step compares the binding affinities of different compounds with the target, and the synthesizing step synthesizes the compound with the highest affinity for the target.

71. The method of claim 41, wherein the integrating step determines an interaction between the compound and the target that indicates the compound binds to the target with an affinity of at least 10^9 M^{-1}.

72. The method of claim 41, wherein the integrating step determines an interaction between the compound and the target that indicates the compound transduces a signal through the target.

73. The method of claim 41, wherein the compounds are potential detergents and the integrating step determines an interaction between the compound and the target that indicates the compound denatures the target.

74. A method of evolving a protein to have a desired functional property comprising:

(a) selecting a model for a reference form of the protein, the model having equations of motion for the protein;

(b) inputting data for an amino acid substitution of the protein into the equations of motions;

(c) integrating said model equations with an L-stable integrator in large time steps so as to obtain a calculation of the motions of the protein with the amino acid substitution;

(d) repeating steps (b) and (c) for additional amino acid substitutions;

(e) comparing the motions of proteins with different amino acid substitutions;

(f) synthesizing a protein with an amino acid substitution selected based on the comparison.

75. The method of claim 74, further comprising testing the selected synthesized protein for a desired functional property.

76. The method of claim 74, wherein the desired functional property is capacity to bind a target.

77. The method of claim 74, wherein the desired functional property is an enzymatic activity.

78. A method of humanizing an immunoglobulin chain, comprising:

(a) providing an amino acid sequence for an immunoglobulin chain comprising CDR regions from a mouse antibody and variable region frameworks from a human antibody;

(b) selecting a model for the immunoglobulin chain the model having equations of motion for the immunoglobulin chain;

(c) integrating the model equations with an L-stable integrator in large time steps so as to obtain a calculation of the motions of the immunoglobulin chain;

(d) determining from the model which amino acid residues in the variable framework region interact with the CDR regions;

(e) substituting one or more of the amino acid residues in the variable framework region that interact with the CDR regions with corresponding amino acids from the mouse antibody;

(f) synthesizing the immunoglobulin chain including the one or more amino acid residues.

79. The method of claim 78, further comprising testing the synthesized immunoglobulin chain for binding to a target.

80. A method of calculating behavior or properties of one or more molecules in specified circumstances, comprising

(a) mathematically modeling said molecules and their environment, said model having equations of motion for said molecules expressed in a reduced set of coordinates; and

(b) numerically integrating said model equations with an implicit integrator using large timesteps, said integrator having stability properties and stepsize selection methods permitting the use of said large timesteps in calculating said behavior or properties with accuracy sufficient for said circumstances.

81. The method of claim 80 wherein said large timesteps comprise an interval of at least 200 femtoseconds.

82. The method of claim 80 wherein said integrating step is performed with varying timesteps.

83. The method of claim 82 wherein said varying timesteps comprise one of at least 200 femtoseconds.

84. The method of claim 80 wherein said stepsize selection method comprises accuracy estimation.

85. The method of claim 80 wherein said stepsize selection method comprises convergence requirements.

86. The method of claim 80 wherein said stepsize selection method comprises energy dissipation requirements.

87. The method of claim 80 wherein said integrator has the L-stability property.

88. The method of claim 80 wherein said integrator comprises an integrator from the group comprising of L-stable members of order 2 or greater of the Radau, SDIRK, SIRK, or Rosenbrock families of integration methods.

89. The method of claim 87 wherein said L-stable integrator comprises the Radau5 integration method.

90. The method of claim 80 wherein said integrator comprises an integrator from the group comprising DASSL and other implicit multistep methods designed for stiff or differential-algebraic systems.

91. The method of claim 80 wherein said coordinates are reduced by the use of one or more rigid bodies comprising two or more atoms each, and internal coordinates.

92. The method of claim 91 wherein the internal coordinates comprise torsion angles.

93. The method of claim 80 wherein said coordinates are reduced by the use of substructuring a molecule into rigid or flexible subcomponents.

94. The method of claim 80 wherein said environment comprises a vacuum.

95. The method of claim 80 wherein said environment comprises a solvent.

96. The method of claim 95 wherein said solvent comprises an implicit representation.

97. The method of claim 96 wherein said implicit solvent comprises non-uniform solvent properties such as membrane regions.

98. The method of claim 80 wherein said circumstances comprise a dynamic simulation.

99. The method of claim 98 wherein said circumstances comprise Newtonian dynamics.

100. The method of claim 98 wherein said circumstances comprise Langevin dynamics.

101. The method of claim 80 wherein said circumstances comprise the search for a reduced energy state of said molecules.

102. The method of claim 101 wherein said search comprises only the local energy basin of the starting configuration.

103. The method of claim 101 wherein said search comprises energy basins other than the local basin of the starting configuration.

104. The method of claim 80 wherein said molecule comprises a single biopolymer in a non-native circumstance, and said properties comprise the folded native structure of said biopolymer.

105. The method of claim 104 wherein said biopolymer is a polypeptide or protein.

106. The method of claim 104 wherein said biopolymer is a nucleic acid.

107. The method of claim 80 wherein said molecules comprise a target molecule and a ligand molecule where said behavior comprises binding of ligand to target or said properties comprise binding affinity, binding preferences, binding rates or other binding properties.